# The study of Nuclear Mass Model by Sequential Least Squares Programming\*

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Nuclear mass is an important property in both nuclear and astrophysics. Some algorithms are applied to improve the accuracy of the nuclear mass model. The algorithm of Sequential Least Squares Programming enhances the precision of multinomial mass models by reducing the error from 1.863 MeV to 1.631 MeV. We further test these algorithms by 200 samples of mass formulas selecting from the  $\delta E$  term of  $E_{isospin}$  mass model. Among these algorithms, the Sequential Least Squares Programming has the best performance in both root mean square errors and computational efficiency. This algorithm is suitable to deal with large-scale, multiparameter optimization tasks in nuclear physics.

Keywords: Nuclear mass model, binding energy, magic nuclei, sequential least squares algorithm

### I. INTRODUCTION

An atomic nucleus contains valuable information about the 3 atomic structure and is a fundamental physical property [1]. 4 Changes in atomic mass directly affect nuclear stability and 5 energy release during nuclear reactions [2]. The mass of a 6 neutron-rich nucleus plays a crucial role in fast neutron cap-7 ture (r-process) during stellar nucleosynthesis. Thus, study-8 ing the mass is essential for a comprehensive understanding 9 of the formation and evolution of elements in the universe 10 [3–5]. Recently, the development of radioactive ion beam fa-11 cilities has led to experimental measurements of over 3000 12 ground state atomic masses [6, 7], with the study continu-13 ously expanding to both sides of the  $\beta$ -stability line. As-14 trophysics requires large amounts of data on the masses of 15 neutron-rich or neutron-poor nuclei in regions far from the 16 stability line. This is difficult to measure directly using cur-17 rent technology. Therefore, many different types of mass 18 models have been proposed.

In 1935, Bethe-Weizsacker proposed the semiempirical 20 BW2 mass formula [8-10] that predicts mass with an accu-21 racy of approximately 3 MeV. In Ref. [11], nuclear binding 22 energy divided into two parts: a large and smooth component along with a small and fluctuating component. The classical droplet model accounts only for the smooth trend and not 25 the rapid fluctuation of the binding energy around the shell 26 gap with a number of protons and neutrons. This suggests that important physical effects are absent in the classical mass 28 model [12, 13]. To solve this problem, physicists have devel-29 oped macroscopic-microscopic mass models. These models 30 introduce shell correction terms, such as the finite force range droplet model (FRDM) [14], Koura-Tachibana-Uno-Yamada 32 (KTUY) [15], Lublin Strasbourg drop (LSD) [16], and mi-33 cromass models such as the Hartree-Fock-Bogoliubov (HFB) 34 approach [17, 18] and relativistic mean-field theory (RMF)

<sup>35</sup> [19]. The cited research is primarily based on the density functional theory (DFT) [20]. Although DFT is more com<sup>37</sup> plex, it exhibits superior extrapolation capabilities.

Kirson et al. added six physical terms as multiple physi-39 cal constraints to the mass model [21–27]. The BW2 mass 40 model thus obtained was solved to some extent, addressing 41 the problems of missing physics and overfitting that existed 42 in early semi-empirical mass formulations, thereby reducing 43 the root mean square error (RMSD) [28] to 1.92 MeV. Ma-44 chine learning has important applications in nuclear physics 45 because of its ability to handle complex problems, such as 46 predicting half-life, charge radius, and charge density [29– 47 32]. By considering the  $\alpha$ -decay energy and Garvey-Kelson 48 relations (GKs) and applying the multi-objective optimiza-49 tion (MOO) method [13, 33, 34], Qian and his research team 50 significantly improved the theoretical accuracy of the BW2 model. Taking into account the isospin dependence, Bhagwat improved the liquid drop model to a model related to isospin and added fluctuation terms [35], which explained the binding energy of nucleons very well. Sequential least squares programming (SLSQP) [36] is a suitable algorithm for solving nonlinear optimization problems with constraints, as it can 57 handle multiple constraints and nonlinear objective functions. 58 SLSQP was initially applied to the layout of antenna arrays. 59 Research has also demonstrated its feasibility and applicabil-60 ity to nuclear mass models.

In this study, we explain the binding energy of nucleons using the improved BW2 mass model by considering the higher-order term of the symmetry energy, which leads to the development of the BW3 mass model [37]. A set of model coefficients for the BW3 mass model was further tested and analyzed using multiple algorithms, aiming to improve the theoretical accuracy and extrapolation ability of the model. In order to verify the universality of the SLSQP algorithm, we applied it to 200 sample mass formulas. The results show that the SLSQP algorithm not only has stability and small root mean square error, but also high computational efficiency. Section 2 introduces the BW3 and  $E_{isospin}$  mass models and sequential least squares programming. Section 3 is the performance of the SLSQP algorithm in enhancing the mass model. Section 4 provides a summary.

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### SEMI-EMPIRICAL MASS FORMULA

#### A. BW3 Mass model

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The mass model of BW3 is derived from the droplet model 79 and improves the semi-empirical mass formula [8–10] by incorporating additional physical constraints[37]:

$$B_{BW3} = \alpha_V A + \alpha_S A^{2/3} + \alpha_C \frac{Z^2}{A^{1/3}} + \alpha_t \frac{(N-Z)^2}{A}$$

$$+ \alpha_{xC} \frac{Z^{4/3}}{A^{1/3}} + \alpha_W \frac{|N-Z|}{A} + \alpha_{st} \frac{(Z-N)^2}{A^{4/3}}$$

$$+ \alpha_p \delta(N, Z) A^{-1/2} + \alpha_R A^{1/3} + \alpha_m P + \beta_m P^2$$

$$+ \alpha_{pm} \frac{(N-Z)^4}{A^3}.$$
(1)

85 Eq.(1) involves 12 parameters, and the  $\delta(N, Z)$  is defined as:

$$\delta(N, Z) = [(-1)^N + (-1)^Z]/2, \tag{2}$$

87 where 1 denotes even-even nuclei, -1 odd-odd nuclei, and 0  $^{88}$  odd-A nuclei. P can be expressed as follows:

$$P = \frac{v_p v_n}{v_n + v_n}. (3)$$

 $_{90}$  Here  $v_{p}\left(v_{n}\right)$  represents the difference between Z (N) and the 91 magic number nearby.

$$\alpha_{pm} = \frac{1}{162} \left( \frac{9\pi}{8} \right)^{\frac{2}{3}} \frac{\hbar^2}{mr_0^2}.$$
 (4)

97 to move freely within the nuclear volume. The potential ex- 135 energy is given by [38] 98 perienced by each nucleon is a superposition of the potenget talls created by other nucleons. Such a system of fermions is regarded as a degenerate gas, with temperatures below the Fermi temperature. The Fermi energy at 0 K is expressed as  $E_p = \begin{cases} \frac{\lambda_n}{N^{1/3}}, & Z \text{ even, } N \text{ odd,} \\ \frac{\lambda_p}{N^{1/3}}, & Z \text{ odd, } N \text{ even,} \\ \frac{\lambda_n}{N^{1/3}} + \frac{\lambda_p}{N^{1/3}} + \frac{\lambda_{np}}{N^{1/3}}, & Z, N \text{ odd,} \end{cases}$ 102 follows:

$$E_F = \frac{h^2}{2m} \left(\frac{3n}{8\pi}\right)^{\frac{2}{3}},\tag{5}$$

where m represents the mass of the fermions, and n means 105 their number density. The Fermi gas model gives the total 139 106 kinetic energy of the nucleons as follows:

$$\begin{array}{ll} {}_{107} & \langle E(Z,N)\rangle \; = \; N\langle E_N\rangle + Z\langle E_Z\rangle \\ \\ {}_{108} & = \; \frac{3}{10m}\frac{\hbar^2}{r_0^2}\left(\frac{9\pi}{4}\right)^{\frac{2}{3}}\left(\frac{N^{\frac{5}{3}}+Z^{\frac{5}{3}}}{A^{\frac{2}{3}}}\right). \end{array} \eqno(6)$$

109 Assuming that the radii of the proton and neutron potential 143 wells are identical, a binomial expansion near N=Z yields 144

111 the following expression:

$$\langle E(Z,N) \rangle = \frac{3}{10m} \frac{\hbar^2}{r_0^2} \left( \frac{9\pi}{8} \right)^{\frac{2}{3}} [A + \frac{5}{9} \frac{(N-Z)^2}{A} + \frac{5}{243} \frac{(N-Z)^4}{A^3} + \cdots].$$
 (7)

114 The first term contributes to the volume in the mass formula, whereas the second corrects for  $N \neq Z$ . The third term rep-116 resents the higher-order addition to the symmetry energy used 117 to enhance the mass model.

### B. $E_{isospin}$ Mass model

The  $E_{isospin}$  mass formula can be expressed by Strutin-120 sky's theorem[35]:

$$E_{isospin}(Z, N) = -(E_{LDM} + \delta E). \tag{8}$$

Here,  $E_{LDM}$  is the macroscopic section and  $\delta E$  represents the fluctuating of the binding energy. The macroscopic sec-124 tion includes the volume term related to the isotopic spin, the 125 Coulomb term, the surface term, the Coulomb energy correc-126 tion term related to surface diffusion and the pairing term:

$$E_{LDM} = \alpha_V \left[ 1 + \frac{4k_V T_z (T_z + 1)}{A^2} \right] A$$

$$+ \alpha_S \left[ 1 + \frac{4k_S T_z (T_z + 1)}{A^2} \right] A^{2/3}$$

$$+ \frac{3Z^2 e^2}{5r_0 A^{1/3}} + \frac{\alpha_C Z^2}{A} + E_p. \tag{9}$$

130 Here,  $a_V$ ,  $k_V$ ,  $a_S$ ,  $k_S$ ,  $a_C$ , and  $r_0$  represent volume en-93 Eq.(4) and its physical terms are derived from the application 131 ergy, isospin dependence of volume energy, surface energy, 94 of the Fermi gas model to account for the nucleon binding en- 132 isospin dependence of surface energy, Coulomb energy, and 95 ergies. Following the restrictions of Pauli's exclusion princi- 133 Coulomb radius, respectively.  $T_Z$  is the third component of  $_{96}$  ple, the nucleons (protons, neutrons, and nuclei) are assumed  $_{134}$  the isospin, and e is the electron charge. The smooth pairing

$$E_{p} = \begin{cases} \frac{\lambda_{n}}{N^{1/3}}, & Z \text{ even, } N \text{ odd,} \\ \frac{\lambda_{p}}{N^{1/3}}, & Z \text{ odd, } N \text{ even,} \\ \frac{\lambda_{n}}{N^{1/3}} + \frac{\lambda_{p}}{N^{1/3}} + \frac{\lambda_{np}}{N^{1/3}}, & Z, N \text{ odd,} \\ 0, & N, Z \text{ even.} \end{cases}$$
(10)

(5)  $^{_{137}}$   $\lambda_n,\lambda_p,$  and  $\lambda_{np}$  are free parameters. The  $\delta E$  can be expressed

$$\delta E(\vec{x}) = \sum_{\vec{k}=\vec{0}}^{\vec{M}} \left\{ a_{\vec{k}} \cos\left(2\pi \frac{\vec{x} \cdot \vec{k}}{M}\right) + b_{\vec{k}} \sin\left(2\pi \frac{\vec{x} \cdot \vec{k}}{M}\right) \right\}. \tag{11}$$

 $= \frac{3}{10m} \frac{\hbar^2}{r_0^2} \left(\frac{9\pi}{4}\right)^{\frac{2}{3}} \left(\frac{N^{\frac{5}{3}} + Z^{\frac{5}{3}}}{A^{\frac{2}{3}}}\right). \quad \text{(6)} \quad \text{$ 

$$x_1 = \beta_1 \left| \frac{N - N_o}{N} \right|, \quad x_2 = \beta_2 \left| \frac{Z - Z_o}{Z} \right|,$$
  
 $x_3 = \beta_3 N^{1/3}, \quad x_4 = \beta_4 Z^{1/3}.$  (12)

 $_{146}$   $\beta_1$ ,  $\beta_2$ ,  $\beta_3$ , and  $\beta_4$  are the free parameters. The  $\beta_1$  and  $\beta_2$  de-  $_{193}$  order necessary conditions: 147 scribe the closeness to a shell closure given proton and neutron conditions, and  $\beta_3$ , and  $\beta_4$  are proportional to Fermi mo-149 mentum. The number of such parameters becomes quite large  $(2M^4+4)$ , while not all terms need to be expanded to M. so 195  $J_g$  and  $J_h$  denote the Jacobian matrices of the equality and it can be simplified as: 151

$$\delta E(\vec{x}) = \sum_{k_1=0}^{M} \sum_{k_2=0}^{M-k_1} \sum_{k_3=0}^{M-k_1-k_2} \sum_{k_4=0}^{M-k_1-k_2-k_3} \left\{ a_{\vec{k}} \cos\left(2\pi \frac{\vec{x} \cdot \vec{k}}{M}\right) + b_{\vec{k}} \sin\left(2\pi \frac{\vec{x} \cdot \vec{k}}{M}\right) \right\}.$$
(13)

 $_{\rm 154}$  It reduces the number of parameters to  $\frac{1}{12}(M+4)!/M! +$ 155 4. Since the mean of  $\delta E$  is almost 0. Therefore, the free parameter can be further reduced to  $\frac{1}{12}(M+4)!/M!+2$ .

#### C. Algorithm Principles

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This work study more than ten algorithms, namely Ordi-158 159 nary Least Squares (OLS) [39], SLSQP [36], Constrained 160 Optimization by Linear Approximation (COBYLA) [40], Broyden-Fletcher-Goldfarb-Shanno (BFGS) [41], Conjugate 161 Gradient (CG) [42], and so on. SLSQP, COBYLA, and Trust-Constr [43] were found to be better effective algorithms for solving constrained optimization problems (COPs). For solving the COP in Eq.(9), SLSQP was used because only SLSQP utilizes the information in the gradient and Hessian matrix [44] to the fullest extent, resulting in faster convergence to 168 the optimal solution.

169 min 
$$f(\vec{x})$$
  
170  $st$   $g(\vec{x}) = 0, h(\vec{x}) \ge 0$   
171  $where$   $\vec{x} = (x_1, x_2, x_3, \dots, x_{k-2}, x_{k-1}, x_k) \in X$   
172  $X = \vec{x} | \vec{l} \le \vec{x} \le \vec{u}$   
173  $\vec{l} = (l_1, l_2, l_3, \dots, l_{i-2}, l_{i-1}, l_i)$   
174  $\vec{u} = (u_1, u_2, u_3, \dots, u_{j-2}, u_{j-1}, u_j).$  (14)

In this formula,  $\vec{x}$  is the solution vector, X is the vector 175 space of solution vectors,  $l(\vec{u})$  is the upper (lower) bounds of the solution vector space,  $g(\vec{x})$  is the equality constraint,  $h(\vec{x})$  is the inequality constraint, and  $f(\vec{x})$  is the objective optimization function [45].

The SLSQP algorithm iteratively minimizes the objec- 223 tive function under constraints through linear approximation. 182 This transforms the nonlinear constrained problem into an un-183 constrained least squares problem. In each iteration, the gradient and Hessian matrix [44] are calculated to update the 227 solution using Lagrange multipliers for the constraints.

$$L(\vec{x}, \vec{\lambda}, \vec{\mu}) = f(\vec{x}) + \vec{\lambda}^T * g(\vec{x}) + \vec{\mu}^T * h(\vec{x}).$$
 (15)

The superscript T denotes the transpose of the vector,  $\vec{\lambda}$  and 232  $\vec{\mu}$  represent the penalty terms associated with the equality and 233 ing RMSD [28], which is defined as follows: inequality conditions, respectively [46].

By solving the unconstrained least squares problem, an up-191 date rule is obtained for each iteration. This rule satisfies not 234

In this formula,  $N_0(Z_0)$  is the magic number nearby. The 192 only the equality and inequality constraints but also the first-

$$\nabla L(\vec{x}, \vec{\lambda}, \vec{\mu}) = \nabla f(\vec{x}) + J_a^T * \vec{\lambda} + J_h^T * \vec{\mu} = 0, \quad (16)$$

inequality constraints, respectively [47].

According to the above update rule, the initial value  $\vec{x}_1$  is 198 chosen and the stopping criterion  $\varepsilon$  is set. The gradient vector 199  $\nabla f_k(\vec{x}_k)$  is computed at each iteration k. If  $||\nabla f_k(\vec{x}_k)|| < \varepsilon$ , 200 the algorithm is terminated, obtaining an approximate solu-201 tion  $\vec{x}^*$ . This process constructs a sequential programming 202 model as follows:

min 
$$q(\vec{x}) = f_k(\vec{x}) + g_k^T(\vec{x} - \vec{x}_k) + \frac{1}{2}(\vec{x} - \vec{x}_k)^T B_k(\vec{x} - \vec{x}_k)$$

$$st \qquad A_{eq}(\vec{x} - \vec{x}_0) = 0$$

$$g_k(\vec{x}) \ge 0, k = 1, 2, \dots, k.$$
(17)

207 In this formula  $B_k$  is a positive definite symmetric matrix 208 used to approximate the inverse of the Hessian matrix, and 209  $A_{eq}$  is the Jacobian matrix of the equality constraints.

This model is solved to obtain the modified direction  $\Delta \vec{x}$ , 211 computing the step size  $\alpha$  such that the objective function 212 sufficiently decreases along the search direction:

$$\alpha = \min(1, r)$$

$$r = \max(\beta_s, r_t)$$

$$\beta_s = \left(\frac{\partial f}{\partial \vec{x}}\right)^T (\Delta \vec{x}/s)$$

$$r_t = \left(\frac{\partial g}{\partial \vec{x}}\right)^T (\Delta \vec{x}/t), \tag{18}$$

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where s and t are positive scale factors. Finally, the estimated points are updated as follows:  $\vec{x}_{k+1} = \vec{x}_k + \alpha \Delta \vec{x}$ . By solving 219 the above system of equations following this iterative process, 220 the objective function is gradually optimized to determine the 221 optimal solution that satisfies the constraints.

## III. DISCUSSION

The coefficients of BW3 model is improved with less 224 error between calculations and data by using SLSQP 225 algorithm[36]. Subsequently, the following constraints are added to ensure the physical feasibility of the program calculations:

- 1. The nuclide numbers should satisfy  $N \ge 8$  and  $Z \ge 8$ .
- 2. After satisfying Condition 1, the specific binding energy (15) 230 of the remaining nuclides,  $\frac{B_{Th}}{N+Z}$ , is distributed in the range of 231 5 - 9 MeV.

The performance metrics of the model were evaluated us-

$$RMSD = \sqrt{\frac{\sum_{i=1}^{n} (B_{Ex_i} - B_{Th_i})^2}{n}},$$
 (19)

TABLE 1.	Coefficients of	of the E	3W3 1	mass	model	under	each	algo-
rithm for bi	inding energy (	(in MeV	V)					

		6 67	`			
	OLS	SLSQP	BFGS	Trust-Constr	L-BFGS-B	CG
$\alpha_V$	16.58	16.05	16.05	16.03	15.19	16.20
$\alpha_S$	-26.95	-23.10	-23.10	-22.96	-16.47	-23.33
$\alpha_C$	-0.774	- 0.74	- 0.74	- 0.74	- 0.71	-0.74
$\alpha_t$	-31.51	-31.62	-31.62	-31.53	-25.83	-31.50
$\alpha_{xC}$	2.22	1.59	1.59	1.59	1.42	1.39
$\alpha_W$	-43.40	-72.96	-72.97	-72.14	5.39	-57.06
$\alpha_{st}$	55.62	64.10	64.10	63.59	23.84	54.80
$\alpha_p$	9.87	10.56	10.56	10.56	12.36	10.63
$\alpha_R$	14.77	9.89	9.89	9.64	- 4.19	9.87
$\alpha_m$	- 1.90	- 1.88	- 1.88	- 1.88	- 1.82	-1.89
$\beta_m$	0.14	0.14	0.14	0.14	0.14	0.14
$\alpha_{pm}$	- 1.30	-11.36	-11.36	-11.31	- 1.13	0.14

 $_{\mbox{\scriptsize 235}}$  where n represents the total number of nuclides involved in the calculation;  $B_{Ex_i}$  and  $B_{Th_i}$  are the current experimental and theoretical nuclide binding energies, respectively.

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The modified coefficients are listed for some algorithms Tab.I The different algorithms change the weights of the 239 in terms in the model, as shown in the table. The weights indicate the extent to which each term affects the model, and the symbols indicate positive or negative corrections. The volume, surface, symmetry, Wigner, surface symmetry, pairing, higher-order correction, and curvature terms have high weights because of their significant influence on the mass model, whereas the Coulomb, Coulomb exchange, and shell effect terms [21–27] have low weights because of their small influence. The horizontal coordinate of the plot is the number of neutrons N, and the vertical coordinate is the percentage of relative error [12] defined as

$$\frac{\delta B}{B}(\%) = \frac{B_{Ex} - B_{Th}}{B_{Ex}} * 100\%.$$
 (20)

The errors exhibit different trends for different nuclide regions under different algorithms. Figs.1-a, 1-b, and 1-c show the reduction in the overall error and narrowing in the fluctuation range of the light and medium nuclide regions. In Figs.1-e and 1-f, the fluctuation amplitude of the heavy nuclide regions is improved, leading to an increase in the fluctuation amplitude of the light nuclide regions, such that the total RMSD does not improve or even deteriorate. SLSQP [36] exhibits greater advantages in reducing model errors when comparing performance metrics such as  $\frac{\delta B}{B}(\%)$  [12] and RMSD [28] of the mass model obtained using different algorithms. This is attributed to the reduced weights of the surface and curvature terms by SLSQP and increased weights of Wigner, surface symmetry, pairing, and higher-order correction terms. The results also showed that in AME2020, the influence of the surface and curvature terms on the binding energy decreases, whereas the influence of the Wigner, surface symmetry, pairing, and higher-order correction terms on the overall effect in- 277

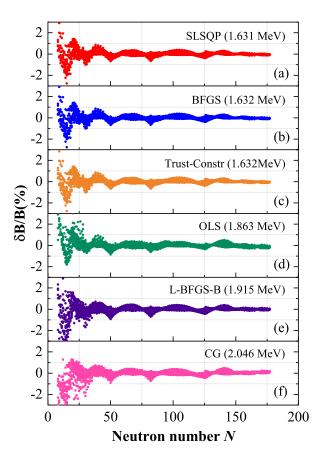
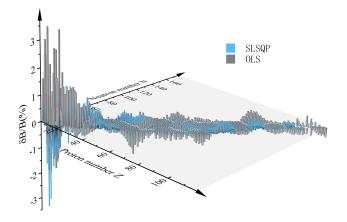


Fig. 1. BW3 mass model relative error comparison using different algorithms, and its RMSD is shown in parentheses.

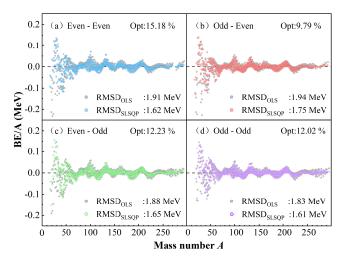
275 SLSQP and more accurately reflects the contributions of the 276 different physical terms to binding energy.



BW3 mass model relative error comparison with SLSQP/OLS coefficients.

Fig.2 shows the relative error between the theoretical creases. This also indicates that the impact of the surface and 278 and experimental values of the BW3 mass model using the 272 curvature terms on the binding energy is reduced, whereas the 279 SLSQP and OLS algorithms, where the x-axis is the neutron 273 impact of the Wigner term on the overall effect increases. The 280 number; the y-axis is the atomic number; and the z-axis is the mass model improves its extrapolation ability [17, 18] under 281 relative error percentage  $\frac{\delta B}{B}$  (%). In the figure, the difference

282 fluctuations are more pronounced for the magic nuclei, espe- 320 speed. 283 cially in the nuclei surrounding the doubly magic nuclei, in- 321 dicating different interactions between magic and non-magic 322 based on the liquid drop model  $E_{LDM}$  with 9 free parameters, <sub>285</sub> nuclei. SLSQP improves the error near the doubly magic nu-<sub>323</sub> and the fluctuation term  $\delta E$ . Setting the degree of freedom M 287 nuclei more accurately, and improves the accuracy of the the-288 oretical model.



BW3 mass model performance on total nuclei with SLSQP/OLS coefficients.

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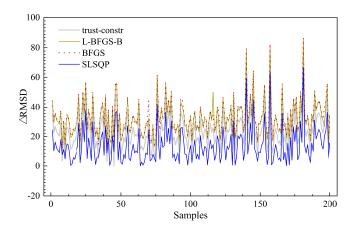
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Fig.3 shows the performance of the SLSQP on even-even, odd-odd, and odd-A nuclei. The optimization effect of SLSQP on the different types of nuclei shows significant differences. The improvement is most significant in the case of even-even nuclei, and some optimization results can also be achieved in the case of odd-A and odd-odd nuclei. Fig.3-a shows that for even-even nuclei [48] (both Z and N are even), SLSQP provides a significant reduction in RMSD [28] by 0.29 MeV, with a performance improvement of about 15.18%, achieving a more substantial optimization in the whole nuclei region compared with the theoretical value of the BW3 model 335 with OLS coefficients. In Fig.3-b, for odd-Z and even-N nuclei, after SLSQP optimization, the model RMSD is reduced by 0.19 MeV, with a performance improvement of approximately 9.79%. Similarly, in Fig.3-c, for even-Z and odddate the effectiveness of SLSQP in mass model optimization. 349 putational efficiency.

The above method are only applicable to one nuclear mass 350 315 formula. In order to verify its universality, we conducted a 351 tween experimental and theoretical values was conducted, as 316 general discussion and applied the method to another multi- 352 illustrated in Fig.5. The experimental binding energy (BE) 317 term nuclear mass formula. The results show that when opti- 353 values were obtained from the AME2020, while the theo-318 mizing the multi-term nuclear mass formula, SLSOP method 354 retical values were predicted by optimizing the BW3 mass

The  $E_{isospin}$  mass model consists of two parts, the 5 terms clei, captures the special interaction effects around the magic 324 to 4, this formula will yield 153 parameters. Referring to the latest nuclear mass dataset AME2020, these parameters are optimized using Ordinary Least Squares (OLS), and the best value of the root mean square deviation is 1.268 MeV.

> By studying the parameters, 62 parameters that have a significant impact on the model were selected. Using these 62 parameters as a sample set, 10 items were randomly selected to form a sample mass formula with the  $E_{LDM}$  item. This random process was repeated to obtain 200 sample mass formulas. Next, we used SLSQP, TRUST-CONST, BFGS and L-BFGS-B algorithms to optimize these mass formulas.



Finding 62 important parameters from the  $\delta E$  term of  $E_{isospin}$  mass model, randomly selecting 10 items as a sample formula with  $E_{LDM}$ , and obtaining 200 samples of mass formulas. The  $\triangle RMSD$  is defined as  $(RMSD - RMSD_{min}) * 100$ , where  $RMSD_{min}$  is the minimum root mean square deviation optimized by the algorithm for 200 samples.

As shown in Fig.4, the SLSQP algorithm is significantly 336 better than the BFGS and L-BFGS algorithms. For example, for the 48th sample point, the  $\triangle RMSD$  of SLSQP is 4 MeV, while that of BFGS and L-BFGS are 23.9 MeV and 23.0 339 MeV respectively. As the 67th sample point, the  $\triangle RMSD$ nuclei, the model RMSD is reduced by 0.23 MeV, with 340 of SLSQP is 2.7 MeV, while BFGS and L-BFGS are 22.7 a performance improvement of approximately 12.23%. No- 341 MeV and 21.8 Mev respectively. For the TRUST-CONSTR tably, in the medium-nuclei region, the optimization results 342 algorithm, there is a large error amplitude which leads to poor are closer to the experimental values. For odd-odd nuclei 343 stability in parameter optimization. In terms of computational (both Z and N are odd), Fig.3-d shows that after SLSQP opti- 344 efficiency compared to the SLSQP algorithm as a reference, mization, the model RMSD is reduced by 0.22 MeV and per- 345 it takes approximately 2.44 times longer in BFGS, 2.78 times 310 formance is improved by approximately 12.02%, particularly 346 longer in L-BFSG-B, and a staggering 8.44 times longer in in the heavy nuclei region, where the optimization results are 347 trust algorithm. The SLSQP algorithm not only has good stacloser to the experimental values. These results further vali- 348 bility with small root mean square errors but also high com-

To verify the effectiveness of the SLSQP, a comparison be-319 performs better with smaller errors and faster convergence 355 model using the SLSQP. Among the experimentally values,

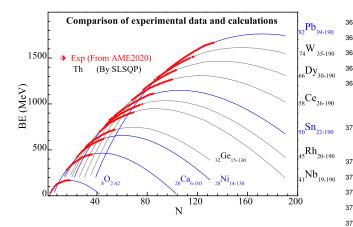


Fig. 5. Binding energy of Exp from the AME2020 [6, 7], and the theoretical predicted value by SLSQP method.

358 decreases as the N increases. The SLSQP-optimized theo- 384 to 1.75 MeV (9.79% optimization). The local RMSD is re-259 retical model predicts the maximum point at <sup>26</sup>O<sub>18</sub> with BE 385 duced from 1.88 MeV to 1.65 MeV (12.23% optimization), = 168.95 MeV, followed by a similar decrease in BE with 386 when proton number is even and neutron is odd. We further <sub>361</sub> increasing N. For the other isotope chains, the experimen-<sub>387</sub> test these algorithms by 200 samples of mass formulas select-362 tally BE values exhibit an overall increasing trend without 388 ing from the  $\delta E$  term of  $E_{isospin}$  mass model. The SLSQP 363 reaching a maximum point. By optimizing the BW3 nuclear 389 shows a small error and fast convergence by comparison with mass model with the SLSQP method, the following BE max- 390 other algorithms.

imum points are predicted for these isotope chains:  $^{64}Ca_{44} =$  $^{366}$  464.33 MeV,  $^{88}Ni_{60}$  = 656.72 MeV,  $^{123}Nb_{82}$  = 950.29 MeV,  $^{141}Rh_{96}$  = 1035.66 MeV,  $^{100}Ge_{68}$  = 745.77 MeV,  $^{156}Sn_{106}$  = 368 1148.31 MeV,  $^{184}Ce_{126}$  = 1311.84 MeV,  $^{206}Dy_{140}$  = 1463.63 369 MeV,  $^{230}W_{156}$  = 1613.36 MeV,  $^{252}Pb_{170}$  = 1761.89 MeV.

#### IV. CONCLUSIONS

In this work, some algorithms are used to improve the accuracy of the mass model BW3. The SLSQP algorithm has the best performance in both root mean square errors and computational efficiency. This algorithm reduces the global RMSD from 1.863 MeV to 1.631 MeV (12.45% reduction). It enhances the precision of multinomial mass models. The odd (even) number of protons and neutrons are discussed, and SLSQP reduces the local RMSD from 1.91 MeV to 1.62 379 MeV (15.18% optimization), when nuclei have even numbers 380 in both protons and neutrons. The local RMSD is reduced 381 from 1.83 MeV to 1.61 MeV, when nuclei have odd numbers 356 the maximum BE for O isotopes is currently measured at 382 in both protons and neutrons. With odd (even) number of pro- $^{24}O_{16}$  with BE = 168.95 MeV. Beyond this point, the BE  $_{383}$  tons (neutrons), the local RMSD is reduced from 1.94 MeV

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